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# The melting transition of a vortex lattice in the uniformly frustrated $XY$ model with quasi-one-dimensional and quasi-two-dimensional coupling anisotropy

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**Abstract**

The uniformly frustrated $XY$ model on the cubic lattice with an anisotropic coupling constant is studied numerically. Quasi-one-dimensional and quasi-two-dimensional systems are examined as models for a charge density wave in a ring crystal and a layer superconductor, respectively. The melting transition of a vortex lattice is investigated by means of non-equilibrium relaxation analysis. We find scaling behaviour of the relaxation with a power law, which indicates that the phase transition is of second order, in contrast to the first-order transition in the isotropic case. The critical exponents are estimated as $\beta = 0.28$ and $z\nu = 2.3$ for the quasi-one-dimensional system and $\beta = 0.40$ and $z\nu = 2.9$ for the quasi-two-dimensional system, and $\alpha \approx 0$ for both cases. This implies that the universality classes of the two are different.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Frustrated systems are among the attractive topics in statistical physics. The uniformly frustrated $XY$ model has been studied as a phenomenological model for high $T_c$ superconductors and Josephson junction arrays under magnetic fields [1, 2]. In the mixed phase between the Meissner and normal phases, the magnetic field penetrates the sample as vortex lines, which are topological defects for the phase of the superconducting order parameter. The case of magnetic field perpendicular to the CuO layer, i.e., parallel to the $c$ axis, has been extensively studied by using the frustrated $XY$ model. It was revealed that the melting transition from the Abrikosov vortex lattice phase to the vortex liquid phase before entering the normal phase is of first order [3]. This is consistent with the experimental results [4].

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The case of transverse field parallel to the CuO layer is attracting more attention [6, 5, 7, 8]. In this case, the quasi-two-dimensional (Q2D) anisotropy of the electronic mobility in the plane perpendicular to the magnetic field plays an important role. Vortex lines are confined between the CuO layers and the vortex core, i.e., the localized normal region, is spreading along the plane. This is called a Josephson vortex. Josephson vortex lines form a triangular lattice which is stretched along the layer direction. The melting transition of a Josephson vortex lattice is predicted to be of second order for sufficiently strong anisotropy in contrast to the isotropic case with the $c$ axis field [5, 8].

Recently the present authors found that charge density waves (CDW) in a ring-shaped crystal of quasi-one-dimensional (Q1D) metal [9, 10] can be mapped onto the frustrated $XY$ model [11]. There, cylindrical bending of the crystal results the frustration between inter-chain and intra-chain couplings and the three-dimensional CDW order realized in usual whisker crystals becomes unstable. This frustration is equivalent to that of the superconductors and the system is regarded as a Q1D superconductor in magnetic field.

In this paper, we numerically investigate the melting transitions of the frustrated systems with strong anisotropy for both Q1D and Q2D cases, paying attention to the continuity and the dimensionality of the phase transitions.

## 2. Model and physical quantities

The Hamiltonian of the uniformly frustrated $XY$ model on a cubic lattice is written as follows:

$$H = \sum_{\alpha=x,y,z} \sum_{\mathbf{i}} J_\alpha \cos(\theta_{\mathbf{i}} - \theta_{\mathbf{i}+\hat{\alpha}} - A_{\mathbf{i},\mathbf{i}+\hat{\alpha}}), \qquad A_{\mathbf{i},\mathbf{i}+\hat{\alpha}} = \begin{cases} 2\pi f i_x & \text{for} \quad \alpha = y \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

Here $\mathbf{i} = (i_x, i_y, i_z)$ is the index of a lattice point and $\hat{\alpha}$ is the unit lattice vector parallel to the $\alpha$ direction. $A_{\mathbf{i},\mathbf{i}+\hat{\alpha}}$ is related to the vector potential on the Landau gauge yielding magnetic field parallel to the $z$ axis. Filling factor $f$ gives the density of vortex lines in the $xy$ plane and is proportional to the magnetic field. The vorticity can be defined at each plaquette: we say that a vortex or anti-vortex exists in a plaquette when the sum of the phase difference along its perimeter is $2\pi$ or $-2\pi$. In three dimensions the vortex line is found by connecting vortices. The anisotropy in the coupling constant is introduced as $(J_x, J_y, J_z) = (\gamma, 1, 1)J_0$ for the Q1D case (chain along the $x$ axis) and $(J_x, J_y, J_z) = (\gamma, 1, \gamma)J_0$ for the Q2D case (layer perpendicular to the $y$ axis) with the anisotropy parameter $\gamma$ much larger than unity.

In the ground state the vortex lines penetrating the sample are straight and parallel to the $z$ axis and they form a lattice in the $xy$ plane. The lattice form depends on $J_x/J_y = \gamma$ only and not on $J_z$, so that Q1D and Q2D systems show the same vortex lattice with the same $\gamma$. This is because the coupling along the $z$ axis is free from the frustration and $\theta$ is uniform in the $z$ direction. As $\gamma$ increases, the vortex lattice is stretched along the $x$ axis and compressed along the $y$ axis with fixed $f$. Finally the distance of vortex lines along the $y$ axis decreases down to the lattice constant of the $y$ axis at a certain value of $\gamma$. Above this $\gamma$ the form of the vortex lattice does not depend on $\gamma$ and the unit lattice vectors are $(\pm 1/2f, 1, 0)$. This crossover is expected to occur around $\gamma \approx \gamma_c(f) = 1/12f^2$ [8].

Since the vortex lines form a two-dimensional lattice, there are Bragg peaks at the reciprocal lattice vectors $\mathbf{q}_v = (\pm\pi f, \pi, 0)$ in the structure factor:

$$S_v(\mathbf{q}) = N|v_z(\mathbf{q})|^2|, \qquad v_z(\mathbf{q}) = N^{-1} \sum_{\mathbf{i}} v_{z\mathbf{i}} e^{i\mathbf{q}\cdot\mathbf{i}}. \tag{2}$$

Here $v_{z\mathbf{i}}$ is a vorticity divided by $2\pi$ defined at the plaquette made by four lattice points, $(i_x, i_y, i_z)$, $(i_x+1, i_y, i_z)$, $(i_x+1, i_y+1, i_z)$, $(i_x, i_y+1, i_z)$. The scalar order parameter is defined as $m = |v_z(\mathbf{q}_v)|$.

The problem we are interested in is the property of the phase transition between the vortex lattice phase and the vortex liquid phase. Equilibrium Monte Carlo simulations of this system are very difficult because of the huge cost of computation. One reason is the slow relaxation dynamics, which is concerned with the trapping in metastable state due to the entanglement of vortex lines. Additionally the system has a large fundamental unit, i.e., a vortex lattice constant, and then very large samples are needed.

In order to avoid this difficulty, we perform non-equilibrium relaxation analysis [12, 13] in a short time on the basis of the scaling hypothesis in the vicinity of the critical temperature $T_c$. When the system is in the ground state at $t = 0$, the order parameter can be scaled as

$$m(\epsilon, t) = \epsilon^{\beta} F(t\epsilon^{z\nu}). \tag{3}$$

Here, $\epsilon = |T - T_c|/T_c$. The critical exponents $\beta$, $\nu$ and $z$ characterize the power law of order parameter $m$, correlation length and relaxation time, respectively. From this scaling, $\beta$ and $z\nu$ can be estimated. Another equation is needed to find the exponents, $z$ and $\nu$, individually. We calculate the fluctuation of the energy per site $e$,

$$f_{ee} = N\left[\frac{\langle e(t)^2\rangle}{\langle e(t)\rangle^2} - 1\right] \sim t^{(2-d\nu)/z\nu} = t^{\alpha/z\nu}, \tag{4}$$

just at $T_c$. The local exponent $\mathrm{d}\ln f_{ee}/\mathrm{d}\ln t$ determines the critical exponent of specific heat, $\alpha = 2 - \mathrm{d}\nu$. Here $\langle\cdots\rangle$ means the ensemble average over the individual runs and $d = 3$ is the dimension of the system.

## 3. Numerical result

In this section, the result of the non-equilibrium relaxation analysis is shown for both Q1D and Q2D anisotropy. The relaxation dynamics at fixed temperature is investigated by means of Monte Carlo simulations with the Metropolis algorithm. The Monte Carlo steps are regarded as time $t$. The initial state is given by the ground state, where

$$\theta_{\mathbf{i}} = (-1)^{i_y}\left[\frac{\pi}{4} - \frac{2\gamma^{-1}}{(2\pi f)^2}\cos(2\pi f i_a)\right] + \mathrm{O}(\gamma^{-2}). \tag{5}$$

This expression is expected from the result of the simulated annealing and variational analysis. The energy of $\mathrm{O}(\gamma^{-2})$ minimized by diffusive dynamics before runs start. We note that there are many degenerate ground states, which are connected to each other by the transformation $\theta \to \theta + 2\pi n i_y/L_y$, $(n = 0, \pm1, \pm2\cdots)$. This transformation conserves vorticity.

### *3.1. Quasi-one-dimensional system*

First, we show the result of the Q1D case. Here filling factor $f$ is chosen to be $1/16$ and $\gamma = 64.0 > \gamma_c(f) = 21.3$. We use the samples with size $L_x \times L_y \times L_z = 512 \times 64 \times 64$. Comparing with a smaller sample of $256 \times 32 \times 32$, a finite size effect is not found in the time range of the simulations. We perform eight independent runs at least for each temperature. The data only for $t > 1000$ are used to get rid of the non-universal behaviour in very short time that does not obey the scaling.

The scaling result obtained by least squares fitting to equation (3) is shown in figure 1. We determine $T_c$, $\beta/z\nu$ and $z\nu$ simultaneously by using the data for $9.70 \leqslant k_B T/J_0 \leqslant 12.0$.

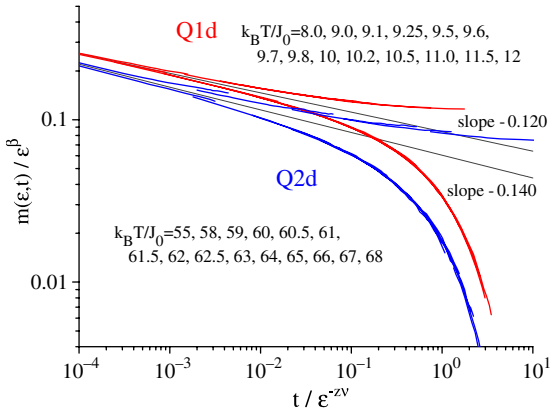


**Figure 1.** Dynamical scaling result for the order parameter. The Q1D and Q2D cases are shown in the same figure. The temperatures are shown in the figure.

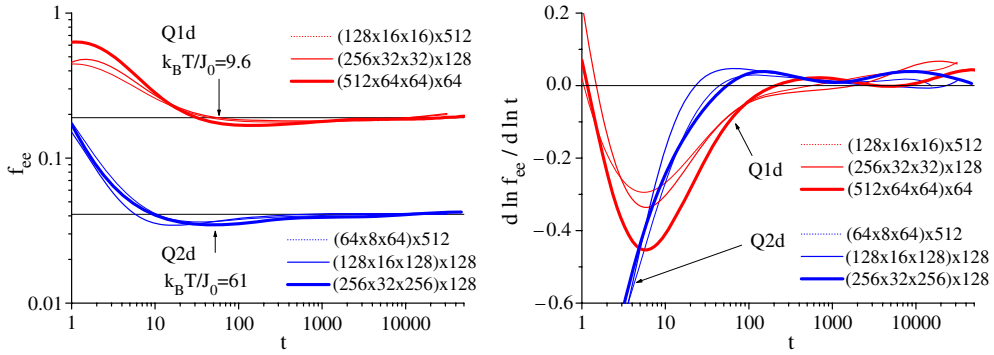


**Figure 2.** The left figure shows the time evolution of the fluctuation of energy per spin, $f_{ee}$, defined in equation (4). The temperatures are 9.6 and $61.0J_0/k_B$. The lines are obtained by smoothing of the data points with local least squares fittings. The sample size and number of samples for averaging are indicated in the legend. The right figure shows the corresponding local exponents.

We can see clear scaling behaviour both above and below $T_c = 9.56J_0/k_B$ with the same critical exponents. Above $T_c$, $m(t)$ exponentially decreases to zero and converges to a finite value below $T_c$. We note that $k_BT_c$ is of the order of $\sqrt{J_xJ_z}$ reflecting the short range phase coherence along the $y$ axis [11].

Figure 2 shows the time evolution of the energy fluctuation at $T = 9.6J_0/k_B \approx T_c$. Within the accuracy of the data, the local exponent $\mathrm{d}\log f_{ee}/\mathrm{d}\log t$ at large $t$ cannot be distinguished from zero. Supposing $\alpha = 0$, $\nu$ equals $2/d = 2/3$ and then $z = z\nu/\nu = 3.5$. There remains a possibility of $\alpha$ being negative, which yields a cusp singularity in the specific heat. This is the case of the ferromagnetic transition of the non-frustrated $XY$ model in three dimensions [14]. Such a singularity cannot be detected by the present method.

### *3.2. Quasi-two-dimensional system*

The conditions of the simulations of the Q2D system are fundamentally the same as those for the Q1D case. The sample size used is $256 \times 32 \times 256$ and the minimum number of runs is 32.

**Table 1.** The list of critical temperatures and exponents.

| | $k_{\mathrm{B}}T_{\mathrm{c}}/\sqrt{J_x J_z}$ | $\beta$ | $z\nu$ | $\nu$ | $z = z\nu/(2/3)$ |
|---|---|---|---|---|---|
| Q1D | 1.20 | 0.28 | 2.3 | (2/3) | 3.5 |
| Q2D | 0.95 | 0.40 | 2.9 | (2/3) | 4.3 |

We set $\gamma = 64$ and $f = 1/16$ in order to compare with the result for the Q1D case, so that the difference is only in $J_z$. This does not change the frustration in the $xy$ plane and therefore the scaling behaviour is almost the same as for the Q1D case as shown in figure 1. In the scaling fitting we use the data for $61.0 \leqslant k_{\mathrm{B}}T/J_0 \leqslant 68.0$. The critical temperature is $61.0J_0/k_{\mathrm{B}}$, which is of the same order as $J_x$ $(=J_z = \sqrt{J_x J_z})$. The exponents are summarized in table 1.

## 4. Discussion

The result in the previous section shows that the Q1D and Q2D systems exhibit qualitatively the same phase transition. This is expected from the fact that there is only a difference in $J_z$ and this has no effect on the ground state. What is important is the breaking of the frustration balance in the $xy$ plane.

The critical behaviour characterized by the power laws indicates that the phase transition is of second order in contrast to the first-order transition for the isotropic case. Such an order change of the phase transition seems peculiar since anisotropy in the coupling constant can usually be removed by proper scaling of the spatial length. But this is not the case for large $\gamma$ because the vortex lattice state which is related to the regular triangular lattice of the isotropic model by such scaling should have a distance between vortex lines in the $y$ direction smaller than the lattice unit, i.e., the spacing of Q2D layers or Q1D chains. Of course this is impossible. Therefore the system with $\gamma \gg \gamma_{\mathrm{c}}(f)$ is essentially different from the isotropic one.

A Kosterlitz–Thouless (KT) phase is proposed for Q2D superconductors [8] but the present result does not agree with this. The structure factor seems to have delta function peaks and the order parameter is $\mathrm{O}(N^0)$ below $T_{\mathrm{c}}$, which indicates true long range order. Additionally the power divergent behaviour of the correlation length ($\xi \propto \epsilon^{-\nu}$) is different from the exponential divergence for the KT transition.

Quantitatively, there are some differences between Q1D and Q2D systems. For example, the critical exponent $\beta$ differs significantly between these cases, which indicates that the universality classes are different. We note, however, that more accurate calculation with larger $\gamma$ is needed to conclude on the difference because the scaling does not work well as $\gamma$ decreases and the error of the critical exponents becomes large. The growth of the relaxation time is slower than the expected power divergence in the very vicinity of the critical point. One possible reason for this is that the structure of the free energy minimum becomes affected by other metastable states, e.g., a vortex lattice state with a lattice constant vector $(\pm 1/4f, 2, 0)$.

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